

in these compounds which are interpreted in terms of perturbed graphitic frequencies.

<sup>1</sup>J. Melin and A. Herold, C. R. Acad. Sc. Paris **269**, 877 (1969)

<sup>2</sup>C. Underhill, S. Y. Leung, G. Dresselhaus, and M. S. Dresselhaus, Solid State Commun. **29**, 769 (1979)

**HH 19 Raman Scattering in Graphite-Lithium Intercalation Compounds.** K.R. SUBBASWAMY, P.C. EKLUND, U. of Kentucky, M.S. DRESSELHAUS, G. DRESSELHAUS, M.I.T., and J.E. FISCHER, Penn. -- The Raman spectra of stage 1 and 2 graphite-lithium intercalation compounds are reported. The spectra show a sharp line at  $\sim 1600 \text{ cm}^{-1}$  near the position of the graphitic optic mode and a broad continuum from  $\sim 1000 \text{ cm}^{-1}$  to  $4000 \text{ cm}^{-1}$  which can be correlated with the two-phonon spectrum of graphite. These spectra are compared to those in other donor and acceptor intercalation compounds.

## SESSION HI: NONMETAL-METAL TRANSITION

Wednesday afternoon, 26 March 1980

Nassau Suite Room A at 2:00 P.M.

J. Wolfe, presiding

**HI 1 Implications of Clustering on the Insulator to Metal Transition in Many Valley Semiconductors.** T. M. RICE and R. N. BHATT, Bell Labs -- The multivalley nature of the conduction bands allows small dense clusters of shallow donors in randomly doped Si and Ge to have a large number of 1s electrons without violating the Pauli principle (12 in Si, 8 in Ge). This leads to large electron affinities of donor clusters, even exceeding the ionization energies of isolated donors. Results based on local density functional calculations of total energy, electron affinity and ionization potential of "jellium" clusters of different sizes and densities will be presented. Implications for the insulator-metal transition in doped many valley semiconductors (e.g., self-compensation and gapless nature of the insulating state) will be discussed.

**HI 2 Anomalous Electrical Resistivity of Barely Delocalized Electrons.** T. F. ROSENBAUM\*, K. ANDRES, G. A. THOMAS, T. M. RICE, and R. N. BHATT, Bell Labs., Murray Hill -- We observe a maximum near 200 K in the zero frequency resistivity of Si:P doped at about twice the Mott density and in the dirty metal limit where the Fermi wave vector times the mean free path is of order 1. The peak indicates a strong T-variation of the screening length, but the T-behavior down to 40 mK shows no evidence of the resistivity minimum predicted<sup>1</sup> for a three-dimensional metal with interference between electron-electron and electron-impurity scattering.

\*Also at Princeton University.

<sup>1</sup>B. L. Altshuler and A. G. Aronov, JETP Letters **27**, 662 (1978).

**HI 3 The Polarizability Enhancement in Doped Semiconductors Near the Metal-Insulator Transition.** D. AGASSI, Univ. of Rochester. -- The averaged polarizability at  $T=0^\circ\text{K}$  due to the randomness in the impurity distribution is evaluated within the one electron-hole (bubble) approximation. The impurity loci are assumed to be Gaussian distributed around an averaged regular array immersed in a uniform dielectric host. The corrections from the randomness add to the bare one-bubble diagram resulting in a modification of the electron/hole propagators and an effective electron hole interaction. These corrections are the leading contributions in the dilute limit ( $N \ll N_c$ ) where  $d \gg a^*$  with  $d$  denoting the averaged lattice constant ( $d \sim N^{-1/3}$ ),  $a^*$  the Gaussian width and  $a^*$  the effective Bohr radius. Based on estimates for (1s, 2p) transition in the polarizability using atomic wave functions, it is concluded that the randomness enhances the polarizability by both reducing the electron-hole energy gap and

mediating electron-hole attraction. The calculated polarizability will be compared with data<sup>1</sup>.

\*Supported in part by US DOE Contract #EY-76-S-02-2171.

<sup>1</sup>T.G. Castner, W.K. Lee, G. Cieloszyk and G. Salinger, Phys. Rev. Lett. **34**, 1622 (1975).

**HI 4 Polarization Catastrophe at an Anderson Transition.** G. A. THOMAS, M. CAPIZZI\*, F. J. DE ROSA, R. N. BHATT and T. M. RICE, Bell Labs., Murray Hill -- We observe a critical enhancement of the electronic polarizability  $\chi$  of a three-dimensional random array of P atoms in crystalline Si in the limits of zero frequency and temperature. We obtain  $\chi$  by Kramers-Kronig analysis of far-infrared spectra of small ( $10^{-4}$  to  $10^{-5} \text{ cm}^{-3}$ ), nominally uncompensated samples at temperatures  $\leq 2 \text{ K}$ . As the P atom density  $n_D$  increases,  $\chi$  rises toward a polarization catastrophe at the insulator-metal transition density  $n_{MI}$  as  $\chi = \chi_0 (1 - n_{MI}/n_D)^{-\zeta}$ , where we find  $\zeta = 1.2 \pm 0.2$  and  $n_{MI} = (4.2 \pm 0.2) \times 10^{18} \text{ cm}^{-3}$ . The observed density  $n_{MI}$  is consistent with other measurements. The exponent  $\zeta$ , however, is much larger than that obtained for classical percolation (.59) emphasizing the quantum mechanical nature of the transition.

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**HI 5 Theory of the Metal-Insulator Transition for Alkali Atoms on a Lattice.\*** J.H. ROSE and L.M. SANDER, U. of Michigan, and H.B. SHORE, San Diego State U. -- The spin density functional theory provides a technique for studying the aspects of the metal insulator (MI) transition due to electron interactions. We systematically study the MI transition for alkali atoms on a periodic lattice. The critical  $r_s$ ,  $[(1/4\pi n)^{1/3}]$ , is found to be  $r_{sc} = (1.03r_0 + 2.8)a_B$ . Here  $r_0$  is the Shaw pseudo-potential radius and  $a_B$  is the Bohr radius. Results are compared with: (1) the MI transition for alkali atoms in a rare gas matrix and (2) gas-liquid critical points. For (1) satisfactory agreement is obtained, while for (2) we find a strong correlation. Additionally we find only a single transition from paramagnetic metal to spin ordered insulator for the entire alkali sequence in contrast to the situation for the MI transition of monatomic hydrogen.

\*Supported in part by the National Science Foundation.

**HI 6 Calculation of the Electrical Conductivity of Liquid Alkali Metal-Gold Alloys.** F. BROUERS, Freie Universität Berlin, W. Germany, CHRISTIANE HOLZHEY, Technische Universität München, W. Germany, and JUDY R. FRANZ, Indiana U. -- The theoretical model developed by Franz, Brouers, and Holzhey<sup>1</sup> to investigate the metal-nonmetal transition in the liquid Cs-Au system, has been applied to the other liquid alkali metal-gold alloy systems. All parameters are taken the same as for the Cs-Au system with the exception of the known alkali metal conduction band widths and electronegativities. It is shown that the model can account for the wide range of behavior found in these systems; <sup>2</sup>Cs-Au and Rb-Au undergo metal-nonmetal transitions near the equiatomic concentration, Na-Au and Li-Au remain metallic at all concentrations, and K-Au exhibits intermediate behavior. Results for the densities of states and charge transfers will be presented as a function of concentration for each alkali-gold system.

<sup>1</sup>J.R. Franz, F. Brouers, and Ch. Holzhey, Journal of Physics F: Metal Physics, to be published.  
<sup>2</sup>N. Nicoloso, R.W. Schmutzler, and F. Hensel, Ber. Bunsenges. Phys. Chem. **82**, 621 (1978).

**HI 7 Metal Insulator Transition in Small Particle Composites,\*** D.M. GRANNAN, J.C. GARLAND, and D.B. TANNER, Ohio State Univ. -- The physics of the metal-insulator transition has been studied in a composite material consisting of Ag particles (approximately 200 Å radius) randomly embedded in a nonconducting KCl medium. Both the electrical conductivity and static